



US007498331B2

(12) **United States Patent**
Gupta et al.

(10) **Patent No.:** **US 7,498,331 B2**
(45) **Date of Patent:** **Mar. 3, 2009**

(54) **ARTHROPOD REPELLENT
PHARMACOPHORE MODELS, COMPOUNDS
IDENTIFIED AS FITTING THE
PHARMACOPHORE MODELS, AND
METHODS OF MAKING AND USING
THEREOF**

5,658,913 A * 8/1997 Kim et al. 514/252.1
6,219,622 B1 4/2001 Schmidt
6,524,605 B1 2/2003 Coats

(75) Inventors: **Raj K. Gupta**, Walkersville, MD (US);
Apurba K. Bhattacharjee, Silver
Spring, MD (US); **Donna Ma Lee**,
Potomac, MD (US)

(73) Assignee: **United States of America as
represented by the Secretary of the
Army**, Washington, DC (US)

(*) Notice: Subject to any disclaimer, the term of this
patent is extended or adjusted under 35
U.S.C. 154(b) by 847 days.

(21) Appl. No.: **10/701,565**

(22) Filed: **Nov. 6, 2003**

(65) **Prior Publication Data**

US 2005/0100575 A1 May 12, 2005

(51) **Int. Cl.**
A01N 43/60 (2006.01)

(52) **U.S. Cl.** **514/252.1**; 424/43; 424/59;
424/69; 424/401; 424/403; 424/405; 424/409;
424/411; 424/412; 424/DIG. 10; 514/844;
514/919; 514/945; 514/953

(58) **Field of Classification Search** 514/252.1
See application file for complete search history.

(56) **References Cited**

U.S. PATENT DOCUMENTS

4,127,672 A 11/1978 Klier
4,707,496 A * 11/1987 Simmons 514/531
4,869,896 A 9/1989 Coulston
4,883,801 A 11/1989 Nathanson
4,946,861 A * 8/1990 Weith et al. 514/436

OTHER PUBLICATIONS

Gouck et al ; R Epellency- J. Econ. Entomol. 50, 175-7 1957.*

Bhattacharjee et al A 3-Dimensional Pharmacophore Model- 129-
AM.J. Trop.Med.Hyg. 67, #2 Suppl. 174-5 2002.*

HCAPLUS abstract# 50:3283f-i, 3284a Gilman et al some
substituted—acids & amides J. of Amer. Chem Soc. 77,6644-6,
1955.*

Dhami, et al Canadian J. of Chemistry, 43(2) 1965—13C NMR
studies.*

International Search Report for PCT/US03/35425, 2 pages.

Arnold WN. (1989) "Evidence of the Pale-Green Liqueur's Toxicity
Eventually Extinguished the Fin-de-Siecle Infatuation with
Absinthe" Sci Am. 260:112-117.

(Continued)

Primary Examiner—Neil Levy

(74) *Attorney, Agent, or Firm*—Elizabeth Arwine

(57) **ABSTRACT**

Disclosed herein is a pharmacophore model for arthropod
repellent activity and methods of making and using thereof.
The pharmacophore comprises two hydrophobic aliphatic
functions, one aromatic function and one hydrogen bond
acceptor function. The pharmacophore model was made
using a test set of arthropod repellent compounds. Also dis-
closed are arthropod repellent compounds identified by
screening databases with the pharmacophore model. Also
disclosed are methods of repelling arthropods from a surface
or area. Compositions and formulations comprising the com-
pounds of the present invention as well as objects having the
compounds of the present invention are disclosed.

8 Claims, 7 Drawing Sheets

